Cobalt-Free Cathodes for Next Generation Lithium-Ion Batteries   Project ID: bat417

Principal Investigator: Neil J. Kidner

NEXCERIS
where energy meets environment

OVERVIEW

Budget

Total Project Funding: $3.08 M

- DOE share: $2.46 M
- Cost share: $620 k
- Funding for FY2020: $1.1 M
- Funding for FY2021: $1.0 M
- Funding for FY2022: $1.0 M

Partners

- Ohio State University: Dr. Jung-Hyun Kim
  Battery testing
  Cell chemistry development
- Navitas Systems Dr. James Dong
  Large-scale electrode fabrication
  2-Ahr battery manufacture and testing

Timeline

- Project Start Date: Jan. 2019
- Project End Date: Mar. 2022
- Percent Complete: 100 %

Barrier and Technical Targets

- Cycle Life: 1000 cycles C/3 deep discharge with < 20 % energy fade
- Cost: < $100/kWh

RELEVANCE

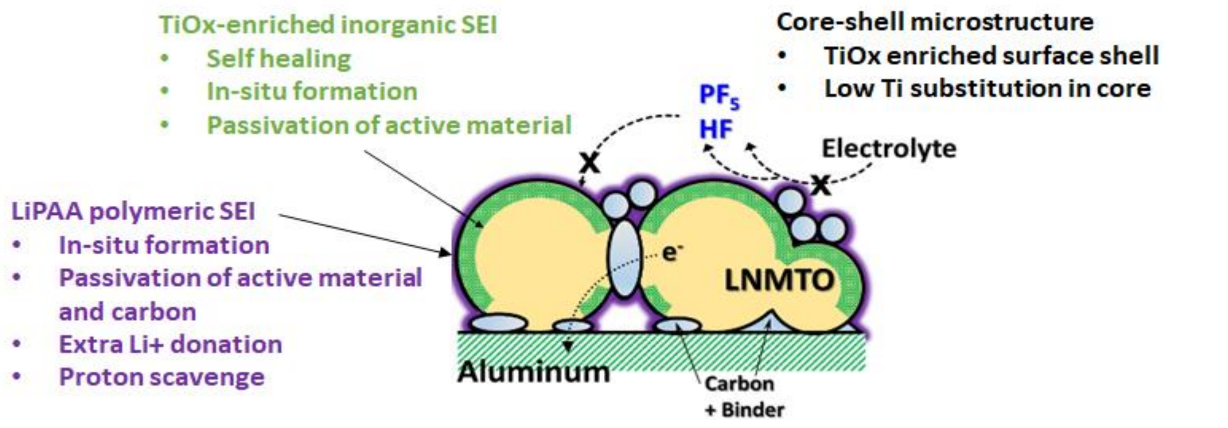
Impact

- The increased demand for EVs is driving demand for battery materials.
- Renewed interest in reduced/cobalt free Li-ion battery cathode formulations
  - Opportunity to reestablish U.S. dominance in batteries

Objective

- Develop high performance and cobalt-free Li-ion battery based on high voltage lithium manganese nickel titanium oxide (LNMTO) cathode and complementary cell chemistry (electrolyte/cathode formulation)
- Identify low-cost, scalable process for producing cathode powder
- Identify strategy for Nexceris to grow domestic manufacturing and create jobs to support new clean energy and e-mobility opportunities

APPROACH



Develop cobalt-free cell based on high-voltage $LiNi_{0.5}Mn_{1.2}Ti_{0.3}O_4$ (LNMTO) cathode

- Improve cycle and calendar life by forming a solid-electrolyte interface that effectively passivates the cathode surface
- Create novel LNMTO core/shell microstructures where Ti is preferentially located at surface and partner with optimized binder/electrolyte chemistries

ACKNOWLEDGEMENTS

Nexceris would like to acknowledge the excellent support of their project partners, Dr. Jung-Hyun Kim at The Ohio State University, and Dr. James Dong at Navitas Systems.

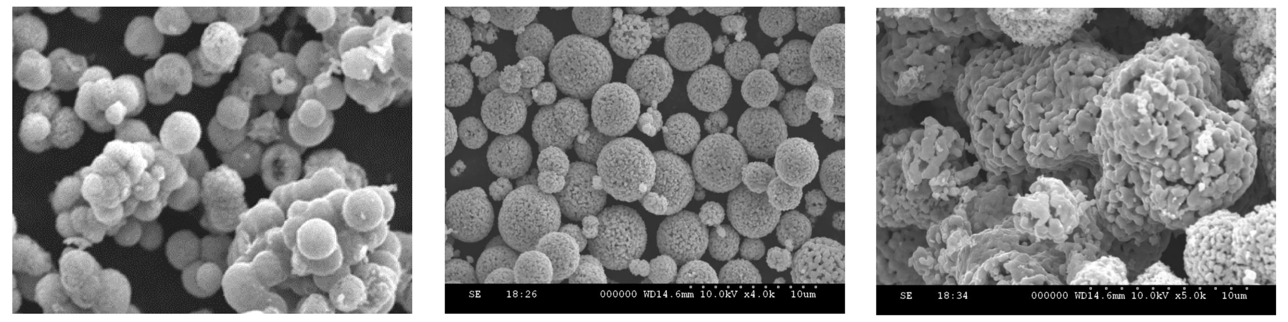
Nexceris would also like to thank the project's DOE Technology Development Manager Dr. Peter Faguy, NETL manager, Adrienne Riggi, and Dr. Jack Deppe and Dr. Ahmad Pesaran for their technical guidance.

This presentation does not contain any proprietary, confidential, or otherwise restricted information

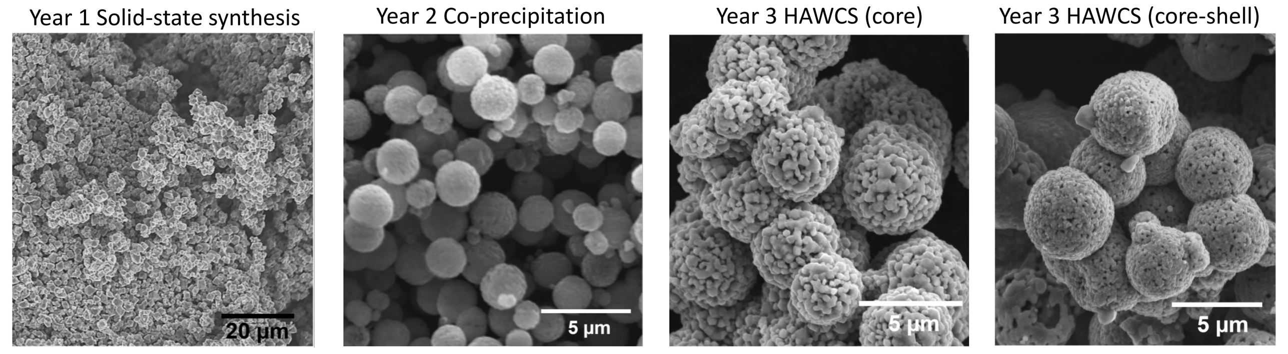
ACCOMPLISHMENT: Core-Shell Cathode Optimization

Building on learnings from Year 2 Intermediate 2-Ah cells the HAWCS synthesis process was refined to optimize the LNMO/LNMTO core-shell microstructure

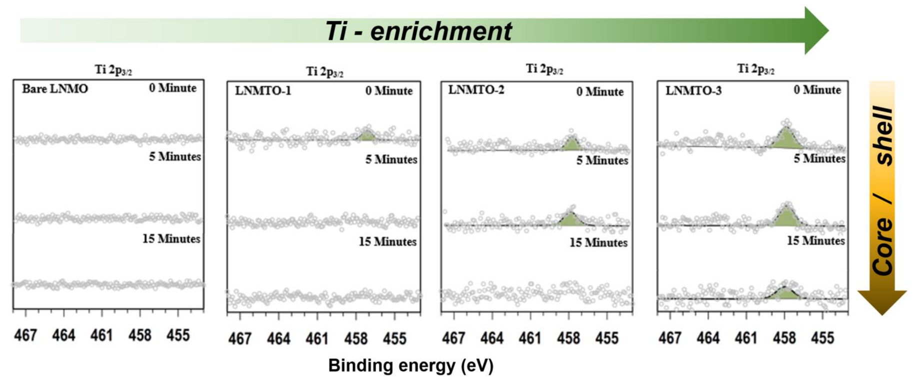
Optimized precipitating agent to transition metal ratio during initial precipitation step
Improved LNMO compositional uniformity resulting in higher capacity



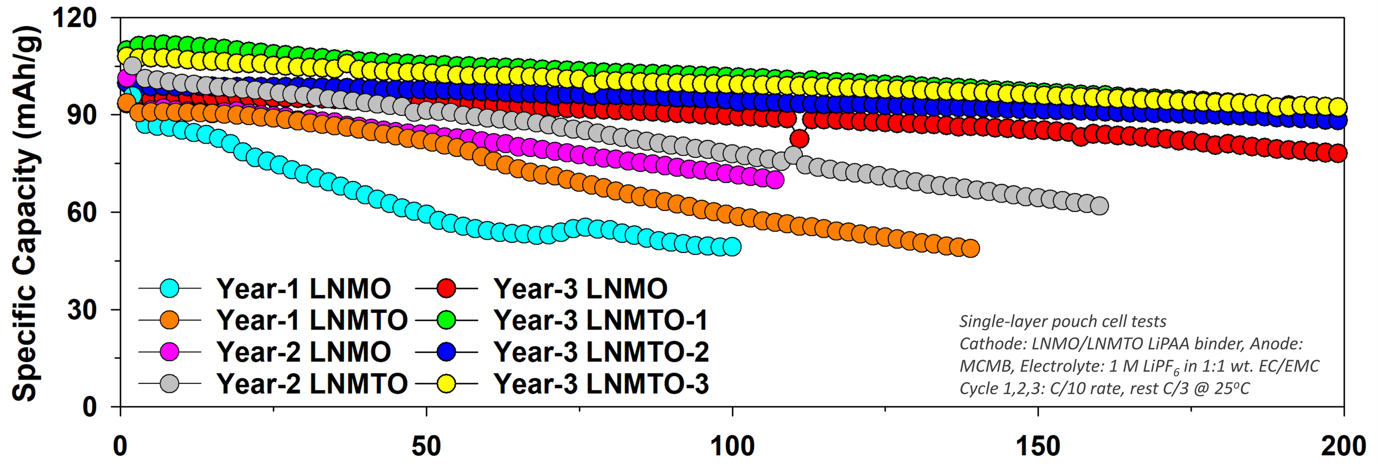
Refined HAWCS synthesis process to target larger diameter core particle
Large core particle reduces surface area and minimizes degradation

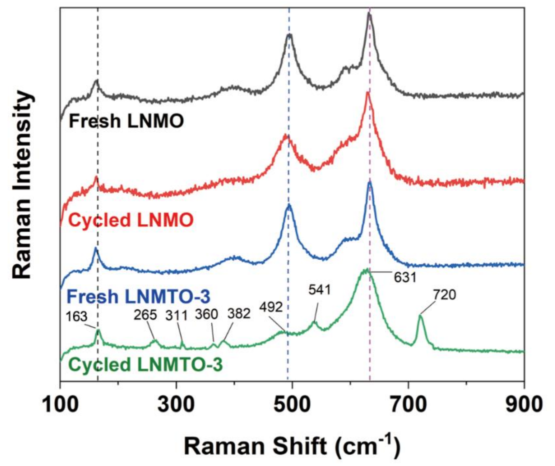


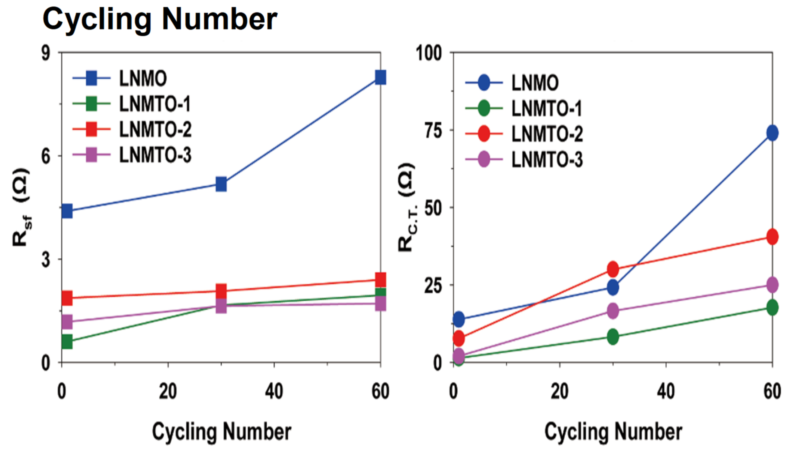
XPS analysis of Year 3 powders Synthesized by HAWCS
Ar-sputtering was performed from 0 – 15 min.
Deeper Ti penetrations with increasing Ti in the shell compositions:
- Bare LNMO: Ti-free
- LNMTO-1: $LiNi_{0.5}Mn_{1.35}Ti_{0.15}O_4$
- LNMTO-2: $LiNi_{0.5}Mn_{1.2}Ti_{0.3}O_4$
- LNMTO-3: $LiNi_{0.5}Mn_{1.0}Ti_{0.5}O_4$



***HAWCS* development provided a systematic improvement in performance for both LNMO core and LNMO/LNMTO core-shell cathodes during the project**







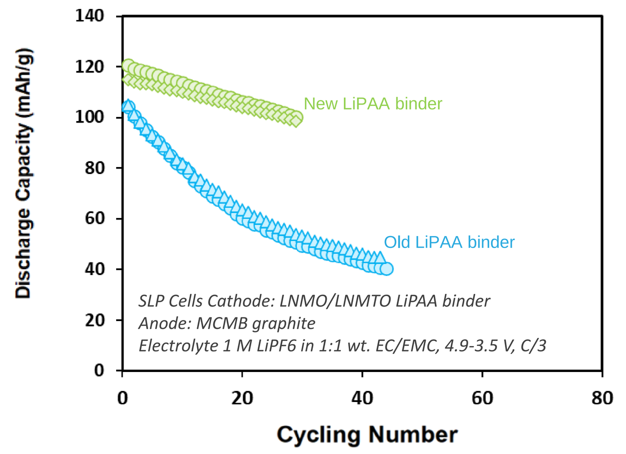
Formation of Ti-rich $LiNi_{0.5}Ti_{1.5}O_4$ was found after cycling LNMTO-3, indicating sacrificial Mn dissolution and formation of the more-stable Ti-enriched CEI layer

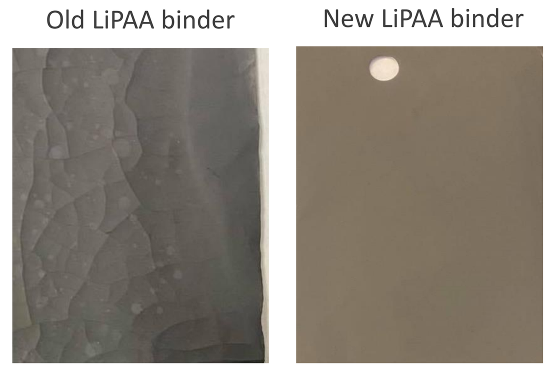
Reduced interfacial impedance (R_{sf}) and charge-transfer (R_{CT}) resistance with Ti-enriched core-shell cathodes in single-layer pouch cells.

ACCOMPLISHMENT: 2 Ah PCC Fabrication and Testing

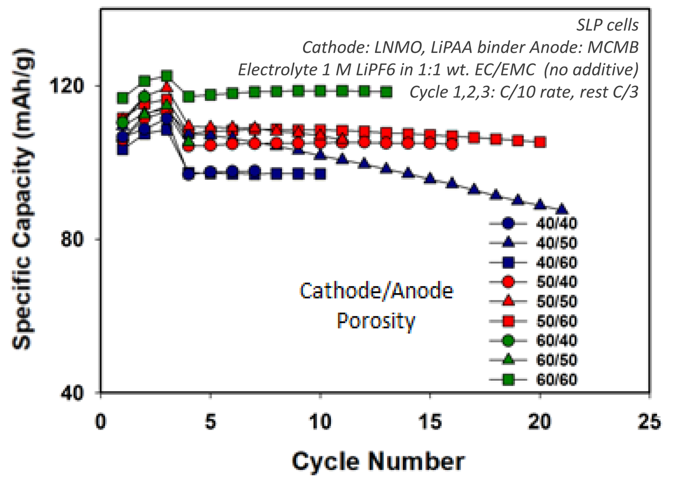
Throughout Year 3 focused on reducing risk through iterative process development to build confidence in scaled powder production larger cell assembly

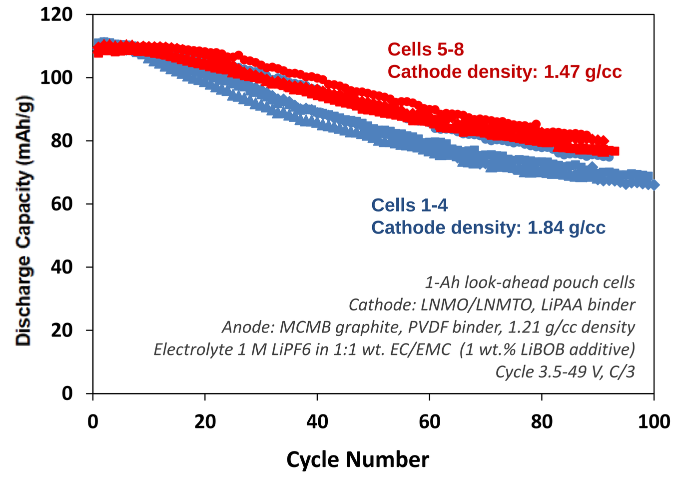
Resolved discrepancy in SLP performance – segmented to LiPAA binder shelf life
Old LiPAA binder makes electrode more susceptible to surface cracks



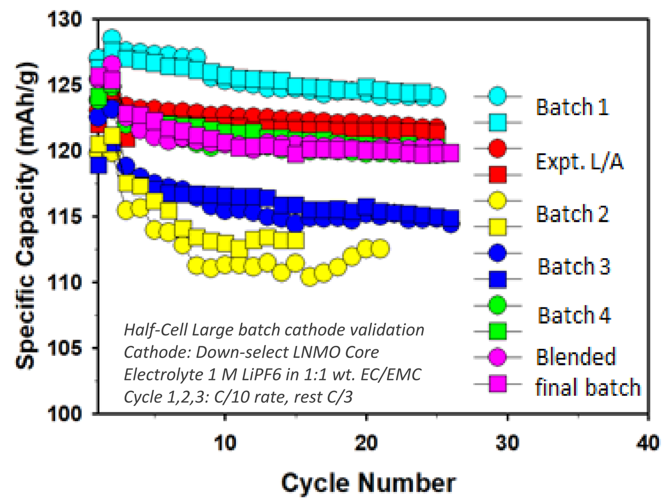


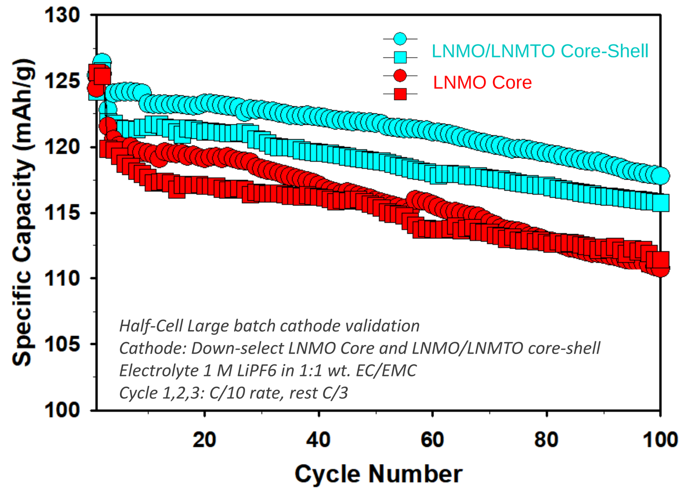
Effect of electrode architecture (density, thickness) studied with SLP cells and lower density (higher porosity) electrodes down-selected



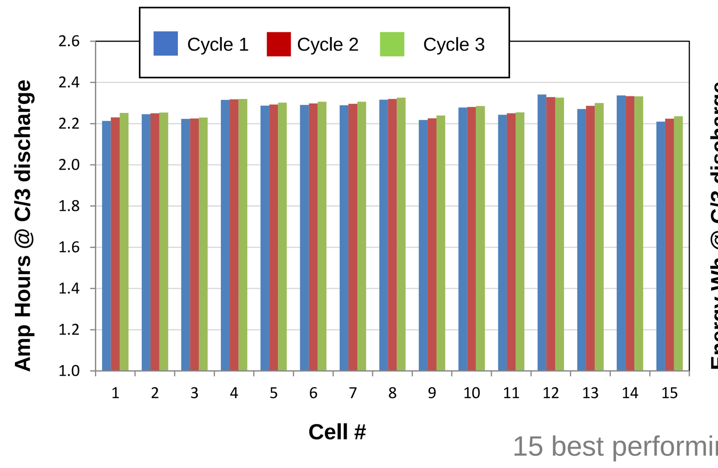


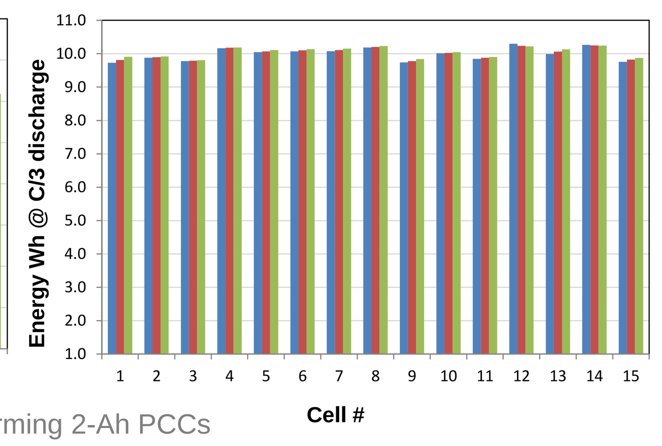
Multiple large LNMO/LNMTO core-shell powder batches produced with excellent batch-to-batch variation





Thirty-four 2-Ah Project Completion Cells (PCCs) successfully fabricated; initial C/3 rated capacity characterized and cells delivered to INL, Navitas and OSU





15 best performing 2-Ah PCCs

MILESTONE REVIEW

Milestone	Metric	Status
Down-select PCC LNMO/LNMTO core shell cathode powder	1. Multiple process refinements completed to optimize the LNMO/LNMTO core/shell powder Down-selection based on 2-Ah cell testing	**Completed** ○ Three LNMO/LNMTO powder iterations completed and PCC powder down selected ○ Cathode powder shipped to Navitas for PCC fabrication
PCC cell chemistry down-selected	1. Define complementary cell chemistry	**Completed** ○ Utilized SLP cell/1-Ah cell formats to identify address cell issues, down-selected cell chemistry/electrode architecture
PCC fabricated	1. Fabricate 30 PCCs to support delivery of 15 to DOE and internal testing.	**Completed** ○ LNMO/LNMTO cathode electrode fabrication completed ○ Thirty-four 2-Ah PCCs successfully fabricated
PCC tested	1. Testing of PCCs at INL and Navitas/OSU	**Completed** ○ Test plan for PCCs finalized with INL ○ PCCs completed C/3 rated capacity/energy cycles ○ Sub-set of cells cycling at Navitas & OSU

COLLABORATIONS/COORDINATION OTHER INSTITUTIONS

Nexceris is fortunate to have excellent project partners that have supported cell chemistry development, testing and large cell (2-Ah) manufacture and testing.

Nexceris has continued to work to engage with stakeholders throughout the Li-ion EV battery value-chain to identify commercial opportunities for developed technology

Project Team Member	Relationship
The Ohio State University	Coin-cell and SLP cell screening of cell chemistries Cell chemistry (additives/binder) development Analytical characterization of cathode materials and electrodes
NAVITAS SYSTEMS	Electrode scale-up, formation-cycling optimization Large format 2-Ahr battery fabrication and testing

PROPOSED FUTURE RESEARCH

Future work should focus on addressing the challenges identified during this project and meeting the commercial performance and cost targets for the material

Gas generation, leading to cell-swelling was identified as a major degradation mechanism for large-format cells. The existing formation cycling procedures were insufficient to prevent gas generation.

- Optimization of formation cycling to minimize gas generation
- Detection of electrolyte leakage from swollen/repaired cells

Further optimization of the complementary electrolyte formulation (additives) for high voltage cathode chemistries is also recommended.

SUMMARY

1. In budget period 3 the project team refined the novel Hybrid Alternative Wet-Chemical Synthesis (*HAWCS*) process for reproducibly producing high-quality LNMO high-voltage cathode powder
2. Three LNMO/LNMTO core-shell powder iterations were completed, and large-batches of powder delivered to Navitas to address scale-up challenges
3. SLP testing identified LiPAA binder shelf-life and electrode architecture (porosity) as critical allowing these parameters to be optimized
4. LNMO/LNMTO cathode powder and cell chemistry down-selected and thirty-four 2-Ah cells fabricated